Data Evaluation Report on the global warming and ozone depletion potential of iodomethane

PMRA Submission Number {.....} EPA MRID Number 45593712

Data Requirement: PMRA Data Code:
EPA DP Barcode: D280800
OECD Data Point:
EPA Guideline: 160-0

Test material: Iodomethane

End Use Product name: **Concentration of a.i.:**
Formulation type:

Active ingredient
Common name: Iodomethane.
Chemical name: Methyl iodide.
IUPAC:
CAS name: Methyl iodide.
CAS No: 74-88-4.
Synonyms:
SMILES string:

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CITATION: Anonymous. October 31, 2000. Estimates of the Atmospheric Lifetime, Global Warming Potential, and Ozone Depletion Potential of Iodomethane (CH_3I). Unpublished study prepared by Atmospheric and Environmental Research, Inc., Cambridge, MA. No study identification number provided. Study submitted by Arvesta Corporation (Tomen Agro, Inc.), San Francisco, CA.

EXECUTIVE SUMMARY:

This study was performed to obtain estimates for the atmospheric lifetime, ozone depletion potential, radiative forcing, and global warming potential for iodomethane.

The study authors utilized some data and information found in studies in compliance with 40 CFR Part 160, Good Laboratory Practices. Other data and information were obtained from non-compliant scientific literature in which a study director was not identified, a study protocol was not developed, and no inspections and reports by a Quality Assurance Unit were performed.

Atmospheric Lifetime of CH_3I

The distribution and lifetime of CH_3I in the atmosphere is a factor of the rate of emission and removal, and is important for determining the build-up of the chemical in the atmosphere. To determine the atmospheric lifetime of CH_3I, estimates of removal [UV absorption cross-section and reaction rate constant of hydroxl (OH)] were obtained from other studies. To simulate the background levels of CH_3I from natural sources (mainly the ocean), a globally uniform surface mixing ratio (3 pptv) was used to obtain a model-calculated atmospheric lifetime for iodomethane of 5.2 days (p. 16). With this lifetime, a flux of 1.7 MT CH_3I/year would be needed to maintain the surface concentration of 3 pptv.

In contrast, the use of CH_3I as a soil fumigant would limit emissions to the northern latitudes. Assuming the same CH_3I emissions, but limited to the northern mid latitudes, the model-calculated atmospheric lifetime for iodomethane was 6.9 days (p. 16).

The two different boundary conditions resulted in variations in the distribution of CH_3I based on the model-calculated concentrations of CH_3I in the troposphere and lower stratosphere. With a uniform mixing ratio boundary, concentrations of CH_3I in the middle troposphere are highest (3 pptv) in the middle and high latitudes due to the faster removal rate in the tropic, mainly from photolysis. When the emission is limited to the northern latitudes, maximum concentration of CH_3I (6 pptv) in the middle troposphere occur in the mid-latitudes of the northern hemisphere. The concentration in the southern hemisphere was very small because most of the CH_3I was removed, mainly by photolysis, before it could be transported across the equator. In both cases, the model-calculated concentration of CH_3I in the upper troposphere was << 0.1% of the surface concentration (p. 16).

Ozone Depletion Potential

The ozone depletion potential (ODP) is the ratio of the ozone depletion produced by a unit-mass of emission of compound X, to the ozone depletion produced by a unit-mass emission of CFC-11 (the traditional reference gas). Ozone depletion is caused by an increase in the concentration of halogen radicals (chlorine, bromine and iodine) in the stratosphere. Photodissociation of CH_3I produces iodine radicals that can reach the stratosphere in two ways: CH_3I can drift into the stratosphere before photodissociation releases iodine radicals (Pathway A), or dissociation can occur in the troposphere and a fraction of the

iodine radicals can be transported into the stratosphere (Pathway B). Because CH_3I is short-lived in the atmosphere, pathway B is more likely because the iodine radicals are released sooner, in the troposphere, rather than the stratosphere, where the ozone layer is located. However, this pathway is also more difficult to predict because the source gas is subjected to small-scale transport in the troposphere, which is not well understood.

To simulate the distribution of I_x, the Atmospheric and Environmental Research's 2-dimensional chemical transport model (AER 2-D CTM) was used. The calculation assumes the soluble I_x species released (HI, HOI and IONO2) are subject to removal by the processes of washout or dry deposition in the troposphere, while the bulk of I_x in the stratosphere is in the form of I and IO. Calculations were performed using the standard washout rate, which has an average first-order removal lifetime of 2 to 10 days, and a deposition velocity of 1 cm/sec.

The study authors defined the empirical ODP by the following equation (pp. 25, 26):

$$ODP^{emp} = ODP(trop) + ODP(stratA) + ODP(stratB)$$

in which,
ODP(*trop*) = ODP of in the troposphere due to I_x accumulation,
ODP (*stratA*) = ODP in the stratosphere due to I_x that are delivered by pathway A,
and ODP(*stratB*) = ODP in the stratosphere due to I_x that are delivered by pathway B.

However, reliable ODP values for CH_3I are difficult to obtain directly from model calculations for two reasons: 1) the model calculations show that the accumulation of I_x in the troposphere leads to ozone depletion in the troposphere, but the model is not capable of resolving variabilities in the troposphere on a regional scale, making the predicted results unreliable. 2) The models have not been tested to determine if they can accurately predict transport of short-lived source gases and their degradation products from the troposphere to the stratosphere.

Estimates of three components of the ODP using a variety of traditional and alternative methods were evaluated. The recommended value was 0.0015 (p. 33) for ODP(*stratA*), which represented the ozone depletion in the stratosphere due to I_x loading via transport of CH_3I (pathway A). This value was derived using traditional well-established methods, including an updated value for the iodine ozone removal efficiency factor using rate constants from JPL-2000 and IUPAC-2000.

Radiative Forcing

Radiative forcing is the ability of a gas to absorb infrared radiation (within the atmospheric spectral window of 750cm-1 and 1300 cm-1), changing the balance of radiation absorbed or emitted by the atmosphere. A gas that strongly absorbs radiation in the atmospheric window, reduces the direct transmission of radiation emitted by the earth to space, enhancing the greenhouse effect (p. 13).

One measure of the effectiveness of a gas to act as a greenhouse gas is the change in radiative forcing at the tropopause (top of the troposphere). Previous studies showed that the calculated change in radiative forcing is proportional to the calculated change in temperature. Using the IR absorption cross-section derived from the absorption data from EPA's Office of Air Quality Planning and Standards (http://www.epa.gov/ttn/emc/ftir/refcas.html), the study author used the AER 1-D RC model to calculate the radiative forcing for CH_3I, assuming that the concentration of CH_3I in the stratosphere was zero (pp. 35 and 38). If the mixing ratio of CH_3I decreased to 5% of its surface value at the tropopause, the radiative forcing was 2.8×10^{-3} Watt m^{-2} per pbbv burden. If the CH_3I was well-mixed, the radiative forcing was 5.0×10^{-3} Watt m^{-2} per pbbv burden. For comparison purposes the radiative forcing for methane (CH_4) and CH_3Br were 5.0×10^{-4} Watt m^{-2} $pbbv^{-1}$ and 1.0×10^{-2} Watt m^{-2} $pbbv^{-1}$, respectively (p. 38).

Global Warming Potential

Global warming potential (GWP) is a relative measure of the warming impact of greenhouse gases, and is defined as the time-integrated warming effect due to an instantaneous release of a unit mass of a given greenhouse gas, relative to that of a reference gas such as carbon dioxide or CFC-11 (p. 14). The measure takes into consideration the infrared absorption characteristics of a gas (computed radiative forcing) and the lifetime of a gas, and compares these to either CFC-11 or carbon dioxide.

The radiative forcing results and a lifetime of 5.2 days were used to calculate the global warming potential (GWP) with different integration time horizons. In the case in which the mixing ratio of CH_3I decreases to 5% of its surface value at the tropopause (radiative forcing is 2.8×10^{-3} Watt m^{-2} $pbbv^{-1}$), the GWP(20), GWP(100) and GWP(500) were calculated to be 0.06, 0.02, and 0.01, respectively. If CH_3I is assumed to be well-mixed (radiative forcing is 5.0×10^{-3} Watt m^{-2} $pbbv^{-1}$), the GWP(20), GWP(100) and GWP(500) were calculated to be 0.11, 0.03, and 0.01, respectively.

The study authors conclude that these values indicate that iodomethane's impact on greenhouse warming is negligibly small (p. 38).